The Claims

1. (Currently Amended) An apparatus comprising:

one or more processors; and

a memory coupled to the processors comprising one or more instructions, the processors operable when executing the instructions to:

determine an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

generate a first set and at least a second set of empirically derived parameters, each set including a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculate a first and second repulsion term of the protein-ligand atom pair according to the first and second sets of empirically derived minimum binding-energy distance and well-depth values, respectively ~~a minimum binding energy distance value and a well-depth value of the atom-pair type~~;

calculate a first and second potential of mean force (PMF) of the protein-ligand atom pair according to the calculated first and second repulsion terms, respectively, ~~term~~ of the protein-ligand atom pair;

calculate a first and second PMF score of the protein-ligand complex according to the calculated first and second PMF of the protein-ligand atom pair, respectively, each ~~the~~ PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex;

predict first and second structures of the protein-ligand complex according to the first and second PMF scores, respectively;

calculate a first root mean square (RMS) deviation between the first predicted structure and an actual, analyzed structure of the protein-ligand complex;

calculate a second root mean square (RMS) deviation between the second predicted structure and the actual, analyzed structure of the protein-ligand complex;

determine agreement between the first set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the first RMS deviation;

determine agreement between the second set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the second RMS deviation; and

communicate at least the PMF score from the first and second PMF scores that is in best agreement with the actual, analyzed protein-ligand atom pair in a user readable format ~~for presentation to a user~~.

2-8 (Canceled)

9. (Currently Amended) The apparatus of ~~Claim 5,~~ Claim 1, wherein one or more of the first set of empirically derived minimum binding-energy distance ~~distances~~ and well-depth values or second sets of empirically derived minimum binding-energy distance ~~distances~~ and well-depth values are each a product of one or more manual processes or automatic processes.

10. (Previously Presented) The apparatus of Claim 9, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

11. (Currently Amended) A method comprising:

determining an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

generating a first set and at least a second set of empirically derived parameters, each set including a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculating a first and second repulsion term of the protein-ligand atom pair according to the first and second sets of empirically derived minimum binding-energy distance and well-depth values, respectively ~~a minimum binding energy distance value and a well depth value of the atom pair type~~;

calculating a first and second potential of mean force (PMF) of the protein-ligand atom pair according to the calculated first and second repulsion terms, respectively ~~term~~ of the protein-ligand atom pair;

calculating a first and second PMF score of the protein-ligand complex according to the calculated first and second PMF of the protein-ligand atom pair, respectively, each ~~the~~ PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex;

predicting first and second structures of the protein-ligand complex according to the first and second PMF scores, respectively;

calculating a first root mean square (RMS) deviation between the first predicted structure and an actual, analyzed structure of the protein-ligand complex;

calculating a second root mean square (RMS) deviation between the second predicted structure and the actual, analyzed structure of the protein-ligand complex;

determining agreement between the first set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the first RMS deviation;

determining agreement between the second set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the second RMS deviation; and

communicating at least the PMF score from the first and second PMF scores that is in best agreement with the actual, analyzed protein-ligand atom pair in a user readable format ~~for presentation to a user~~.

12-18 (Canceled)

19. (Currently Amended) The method of ~~Claim 15,~~ Claim 11, wherein one or more of the first set of empirically derived minimum binding-energy distance ~~distances~~ and well-depth values or second sets of empirically derived minimum binding-energy distance ~~distances~~ and well-depth values are each a product of one or more manual processes or automatic processes.

20. (Previously Presented) The method of Claim 19, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

21. (Currently Amended) Software encoded in one or more computer-readable tangible media and when executed operable to:

determine an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

generate a first set and at least a second set of empirically derived parameters, each set including a minimum binding-energy distance value and a well-depth value of the atom-pair type;

calculate a first and second repulsion term of the protein-ligand atom pair according to the first and second sets of empirically derived minimum binding-energy distance and well-depth values, respectively ~~a minimum binding energy distance value and a well depth value of the atom pair type~~;

calculate a first and second potential of mean force (PMF) of the protein-ligand atom pair according to the calculated first and second repulsion terms, respectively, ~~term~~ of the protein-ligand atom pair;

calculate a first and second PMF score of the protein-ligand complex according to the calculated first and second PMF of the protein-ligand atom pair, respectively, each ~~the~~ PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex;

predict first and second structures of the protein-ligand complex according to the first and second PMF scores, respectively;

calculate a first root mean square (RMS) deviation between the first predicted structure and an actual, analyzed structure of the protein-ligand complex;

calculate a second root mean square (RMS) deviation between the second predicted structure and the actual, analyzed structure of the protein-ligand complex;

determine agreement between the first set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the first RMS deviation;

determine agreement between the second set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the second RMS deviation; and

communicate at least the PMF score from the first and second PMF scores that is in best agreement with the actual, analyzed protein-ligand atom pair in a user readable format ~~for presentation to a user~~.

22-28 (Canceled)

29. (Currently Amended) The software of ~~Claim 21,~~ Claim 25, wherein one or more of the first set of empirically derived minimum binding-energy distance ~~distances~~ and well-depth values or second sets of empirically derived minimum binding-energy distance ~~distances~~ and well-depth values are each a product of one or more manual processes or automatic processes.

30. (Previously Presented) The software of Claim 29, wherein at least one of the automatic processes comprises execution of a genetic algorithm.

31. (Currently Amended) A system comprising:

means for determining an atom-pair type of a protein-ligand atom pair in a protein-ligand complex;

means for generating a first set and at least a second set of empirically derived parameters, each set including a minimum binding-energy distance value and a well-depth value of the atom-pair type;

means for calculating a first and second repulsion term of the protein-ligand atom pair according to the first and second sets of empirically derived minimum binding-energy distance and well-depth values, respectively ~~a minimum binding-energy distance value and a well-depth value of the atom-pair type~~;

means for calculating a first and second potential of mean force (PMF) of the protein-ligand atom pair according to the calculated first and second repulsion terms, respectively ~~term~~ of the protein-ligand atom pair;

means for calculating a first and second PMF score of the protein-ligand complex according to the calculated first and second PMF of the protein-ligand atom pair, respectively,

each ~~the~~ PMF score indicating a binding affinity between a protein and a ligand in the protein-ligand complex;

means for predicting first and second structures of the protein-ligand complex according to the first and second PMF scores, respectively;

means for calculating a first root mean square (RMS) deviation between the first predicted structure and an actual, analyzed structure of the protein-ligand complex;

means for calculating a second root mean square (RMS) deviation between the second predicted structure and the actual, analyzed structure of the protein-ligand complex;

means for determining agreement between the first set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the first RMS deviation;

means for determining agreement between the second set of empirically derived minimum binding-energy distance and well-depth values and the actual, analyzed protein-ligand atom pair based at least in part on the second RMS deviation; and

means for communicating at least the PMF score from the first and second PMF scores that is in best agreement with the actual, analyzed protein-ligand atom pair in a user readable format ~~for presentation to a user~~.